Coupling of MD with Continuum Mechanics via a Bridging Scale Approach

Multiscale Simulation Methods Workshop

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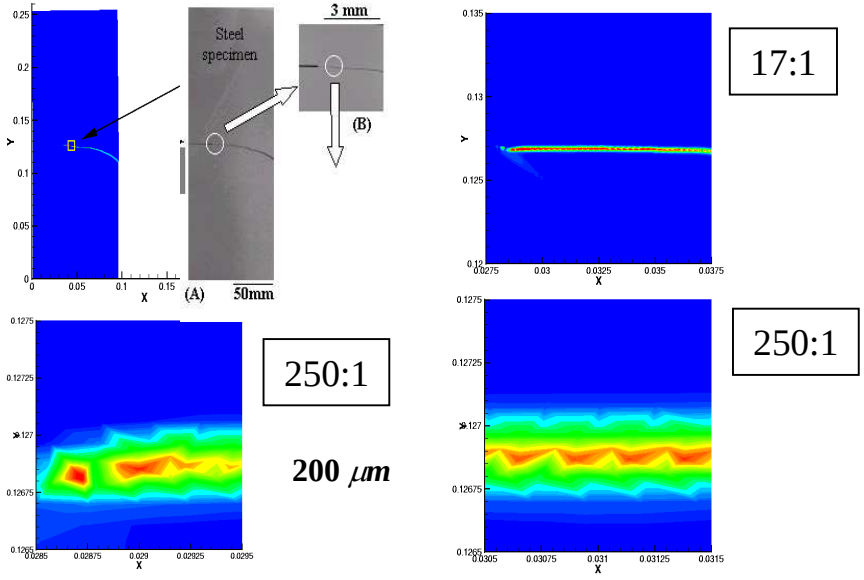
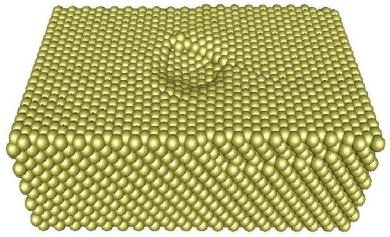
Examples of Multi-Scale Phenomena in Solids

Fracture/Failure of Solids



Prof. Shaofan Li, U.C.-Berkeley

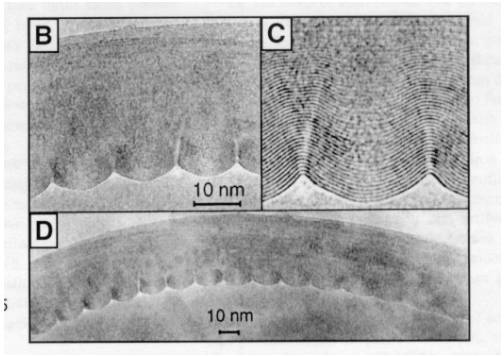
Nanoindentation



Dr. Eduard Karpov, Northwestern University

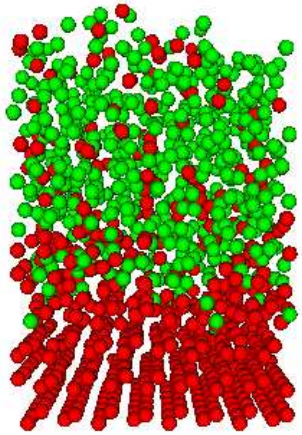
Nanoscale Devices

Poncharal et al., *Science* **283**:1513



Prof. Dong Qian, U. of Cincinnati

Film Growth



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Concurrent Multiscales: Motivation

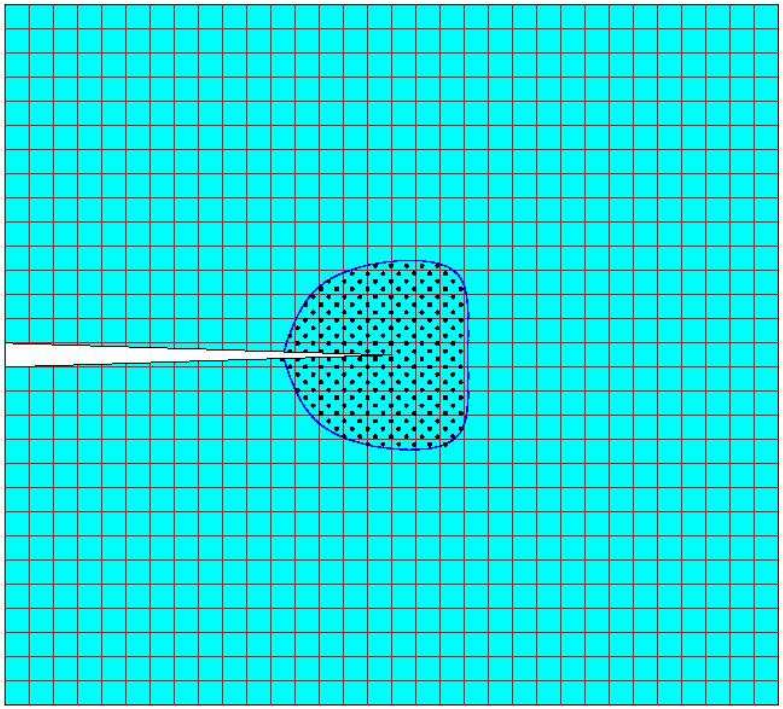
- Molecular dynamics simulations are limited to small domains (~10^6-10^8 atoms) and small time frames (~nanoseconds)
  - Experiments, even on nano-systems, involve much larger systems over longer times
- Continuum models are good, but not always adequate
  - Problems in fracture and failure of solids require improved constitutive models to describe material behavior
  - Molecular dynamics is required in regions of high deformation or discontinuity
- Multiple scale nature of these problems calls for a combined molecular dynamics/continuum mechanics approach

Concurrent Multiple Scales: Goals

- Method for coupling molecular dynamics to finite element or meshfree computations in concurrent simulations
  - Simulation of time dependent, finite temperature problems
- True “coarse scale” discretization in continuum
  - No meshing down to atomic scale
  - Subcycling time-stepping algorithms to take advantage of multiple time scales
    - don’t want to be limited to nano time scale everywhere in the domain
- Easy implementation
  - Re-use of existing MD and continuum codes
  - Easily parallelizable algorithms

Concurrent Coupled Simulations

- Molecular dynamics to be used in region of interest
  - near crack/shear band tip
  - inside shear band
  - at area of large deformation
  - around dislocations
  - etc.
- Finite elements/meshless “coarse scale” defined *everywhere* in domain
  - not just overlap/handshake region
- Bridging scale used to ensure FEM gives correct coarse scale behavior



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2-Part Strategy for Multiscale Coupling

- First, formally define exactly what is simulated at each scale
  - decompose total solution into coarse and fine scales
  - “bridging scale” used to represent the part of the total solution common to both simulations
    - provides coupling between the two simulations
- Second, eliminate fine scale degrees of freedom analytically outside of region of interest
  - use molecular dynamics (MD) only where necessary
  - use bridging scale decomposition to further define coupling between simulations
    - constitutive law in pure coarse scale region
    - boundary conditions on MD region

Coarse-Fine Decomposition

- Fields like displacement are decomposed into coarse and fine scales:

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$$

- Coarse scale is represented by smooth basis functions associated with nodes, e.g. finite element shape functions:

$$\bar{\mathbf{u}}(\mathbf{X}_\alpha) = \sum_I N_I(\mathbf{X}_\alpha)\mathbf{d}_I \xrightarrow[\text{notation}]{\text{matrix}} \bar{\mathbf{u}} = \mathbf{N}\mathbf{d}$$

  - nodal degrees of freedom minimize mass-weighted error norm:

$$E = (\mathbf{u} - \mathbf{N}\mathbf{d})^T \mathbf{M}_A (\mathbf{u} - \mathbf{N}\mathbf{d})$$

$$\frac{dE}{d\mathbf{d}} = 0 \Rightarrow \mathbf{d} = (\mathbf{N}^T\mathbf{M}_A\mathbf{N})^{-1}\mathbf{N}^T\mathbf{M}_A\mathbf{u}$$

  - This leads to a definition of the coarse scale in terms of a projection matrix:

$$\boxed{\bar{\mathbf{u}} = \mathbf{P}\mathbf{u}}$$

$$\mathbf{P} = \mathbf{N}(\mathbf{N}^T\mathbf{M}_A\mathbf{N})^{-1}\mathbf{N}^T\mathbf{M}_A$$

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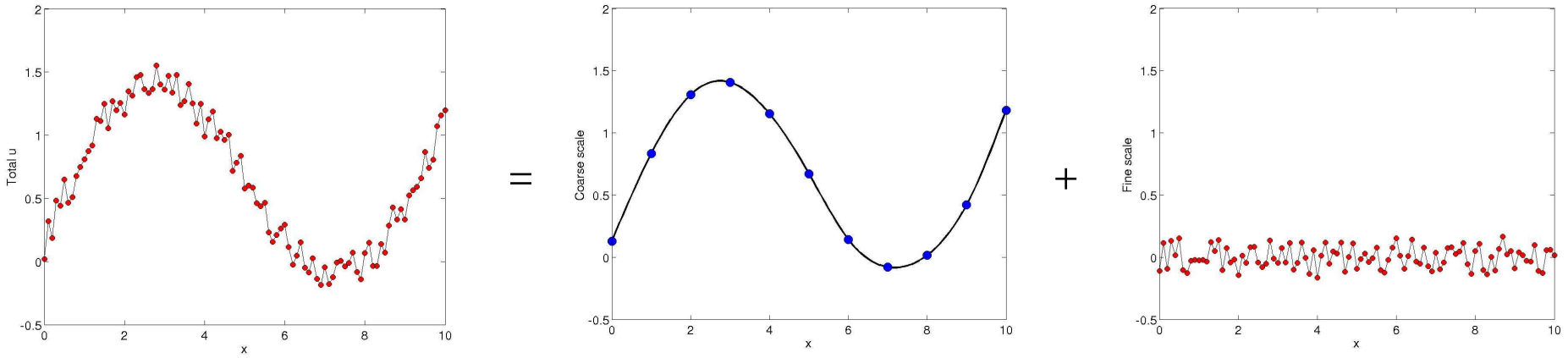
Coarse-Fine Decomposition

- Once coarse scale is defined, fine scale is “everything else”:

$$\begin{aligned} \mathbf{u}' &= \mathbf{u} - \bar{\mathbf{u}} \\ &= \mathbf{u} - \mathbf{P}\mathbf{u} \\ &= (\mathbf{I} - \mathbf{P})\mathbf{u} \equiv \mathbf{Q}\mathbf{u} \end{aligned}$$

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$$



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Concurrent Multiscale Solution

- Use FEM for the coarse scale, MD for the fine scale in the decomposition:

$$\bar{\mathbf{u}} = \mathbf{N}\mathbf{d} \longrightarrow \text{solve } \mathbf{d} \text{ using FEM}$$

$$\mathbf{u}' = (\mathbf{I} - \mathbf{P})\mathbf{q} \longrightarrow \text{solve } \mathbf{q} \text{ using MD}$$

- With our choice of projection operator, kinetic energy separates completely into coarse and fine scales:

$$K_E = \frac{1}{2}\dot{\mathbf{d}}^T \mathbf{M}\dot{\mathbf{d}} + \frac{1}{2}\dot{\mathbf{q}}^T \tilde{\mathbf{M}}\dot{\mathbf{q}}$$

- Coupling between scales is only through the forcing term
  - Final momentum equations become:

$$\begin{aligned} \text{Coarse scale:} \quad & \mathbf{M}\ddot{\mathbf{d}} = \mathbf{N}\mathbf{f}(\bar{\mathbf{u}} + \mathbf{u}') \\ \text{Fine scale:} \quad & m_\alpha \ddot{\mathbf{q}}_\alpha = \mathbf{f}_\alpha(\bar{\mathbf{u}} + \mathbf{u}') \end{aligned}$$

Reference: G. Wagner and W.K. Liu, *JCP* **190**:249-74 (2003).

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Coarse Scale Modeling

- Coarse scale equation can be related to usual finite element treatment by approximating summations over atoms as domain integrals:

$$\sum_J \mathbf{M}_{IJ}\ddot{\mathbf{d}}_J = \mathbf{f}_I\left(\bar{\mathbf{u}}, \mathbf{u}'\right)$$

where

$$\mathbf{M}_{IJ} = \int_\Omega \rho(\mathbf{x}) N_I(\mathbf{x}) N_J(\mathbf{x}) d\mathbf{x}$$

- The nodal force depends on the coarse scale only through the deformation gradient **F:**

$$\begin{aligned}\mathbf{f}_I &= -\frac{\partial U}{\partial \mathbf{d}_I} \\ &= -\sum_\alpha \frac{\partial W_\alpha}{\partial \mathbf{d}_I}\Delta V_\alpha \\ &= -\sum_\alpha \frac{\partial \mathbf{F}_\alpha}{\partial \mathbf{d}_I}\frac{\partial W_\alpha}{\partial \mathbf{F}_\alpha^T}\Delta V_\alpha \approx -\int_\Omega N_{I,\mathbf{x}}(\mathbf{x})\mathbf{P}^K(\mathbf{x})dV\end{aligned}$$

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Fine Scale Boundary Conditions

- We want to avoid grading the coarse mesh down to the atomic lattice scale at the boundary
  - expensive
  - too much information
  - limits coarse scale time step
- Information passes from a fine MD lattice directly into a coarse scale mesh
  - small-scale energy can't be represented on the coarse scale, has nowhere else to go
  - leads to **internal reflection** of small scale waves
- Proper boundary treatment requires accounting for fine scale dynamics that are not simulated directly
  - correct boundary treatment falls out automatically from bridging scale decomposition
    - linearize in the fine scales at the boundary

MD Boundary Condition

$$\ddot{\mathbf{q}}_1(t) = \mathbf{M}_A^{-1}\mathbf{f}_1^*(t) + \int_0^t \boldsymbol{\theta}(t-\tau)\mathbf{a}_2'(\tau)d\tau + R_1(t)$$

$$\mathbf{a}_2'(t) = \mathbf{M}_{A2}^{-1}\mathbf{f}_2^*(t) - \ddot{\bar{\mathbf{u}}}_2(t)$$

Region 1: MD + FEM
Region 2: FEM only (+ "ghost atoms")

where $\mathbf{f}^*(t)$ are forces computed using just the coarse scale displacements outside MD region (e.g. through "ghost atoms")

- The total forcing term consists of three major parts:
  - The standard interatomic force computed in MD simulation by assuming displacements of all atoms just outside the boundary are given by the coarse scale
  - A time history-dependent dissipation at the boundary (similar to a damping term)
  - A random forcing term at the boundary
    - the form of this term can be related to the temperature of the solid:

$$\langle R_i(t)R_j(0)\rangle = -\delta_{ij}\beta(t)k_BT$$

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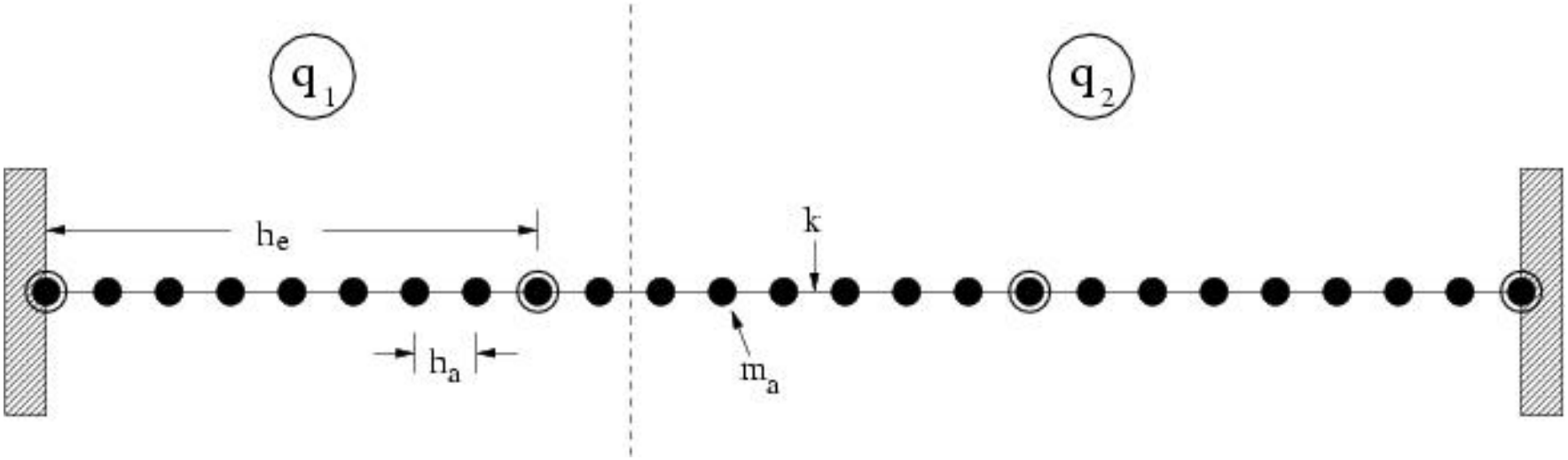
Example Problem: 1D Harmonic Chain



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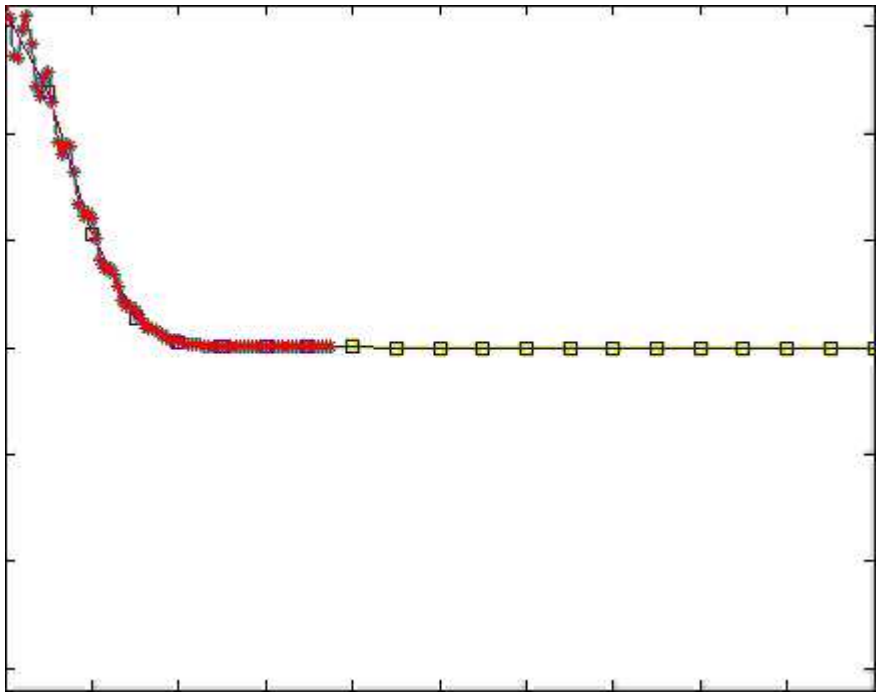
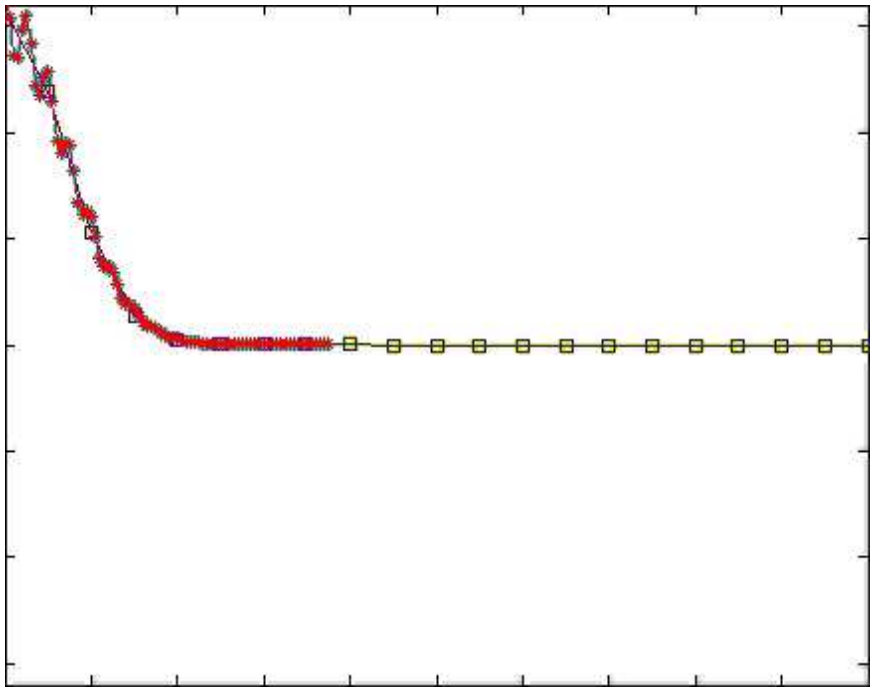
Effects of BC's on Internal Wave Reflection

$$\dot{\mathbf{q}}_\alpha = \sum_I N_I(\mathbf{x}_\alpha)\dot{\mathbf{d}}_I$$

$$\ddot{\mathbf{q}}_1(t) = \mathbf{M}_A^{-1}\mathbf{f}_1^*(t) + \int_0^t \boldsymbol{\theta}(t-\tau)\mathbf{a}_2'(\tau)d\tau$$





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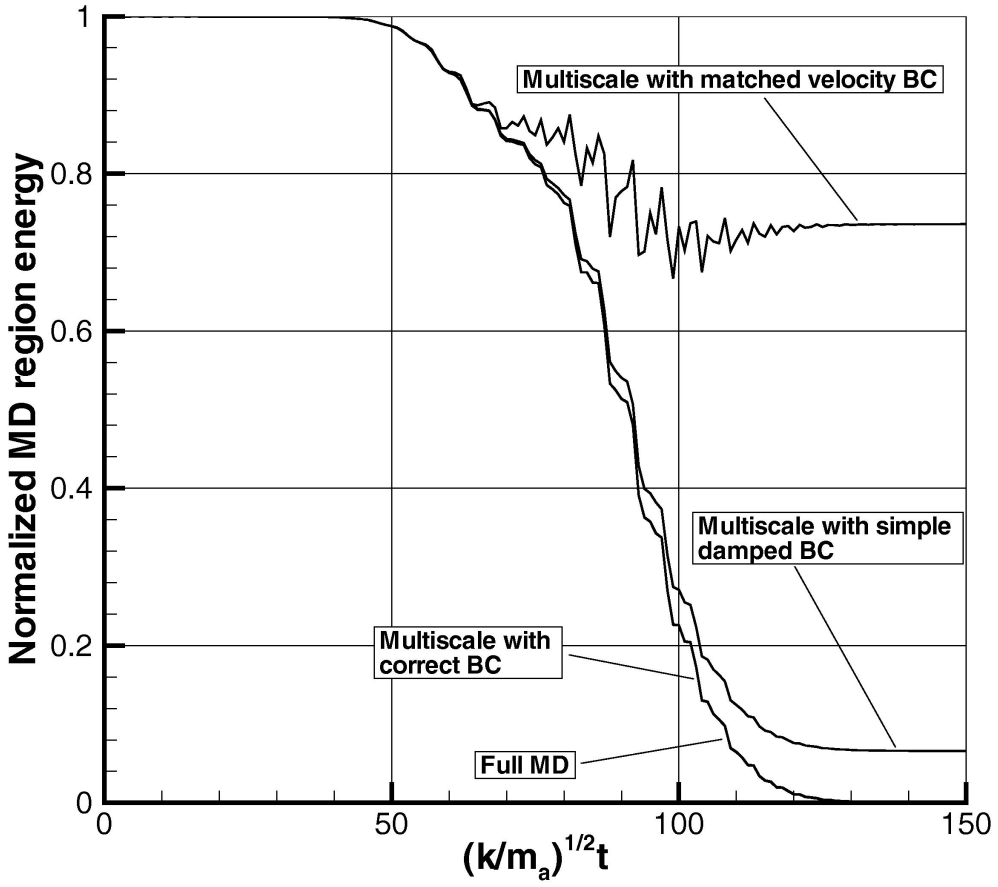
Energy Transfer out of MD Region



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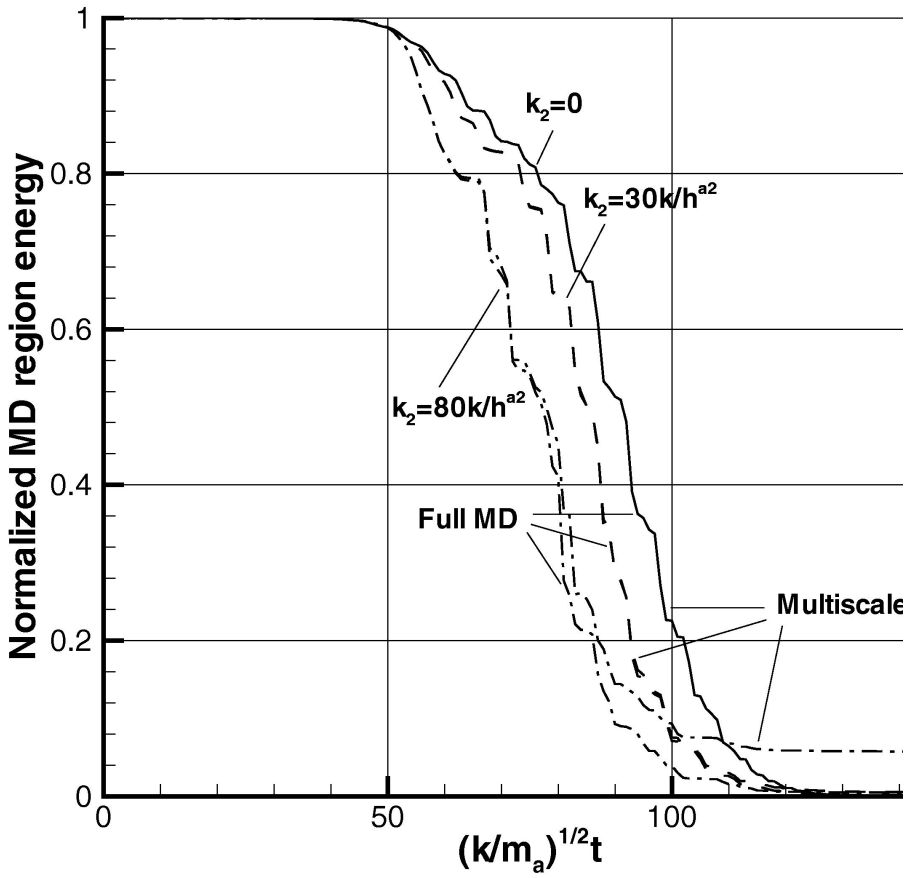
Energy Transfer out of MD Region: Nonlinear Potential



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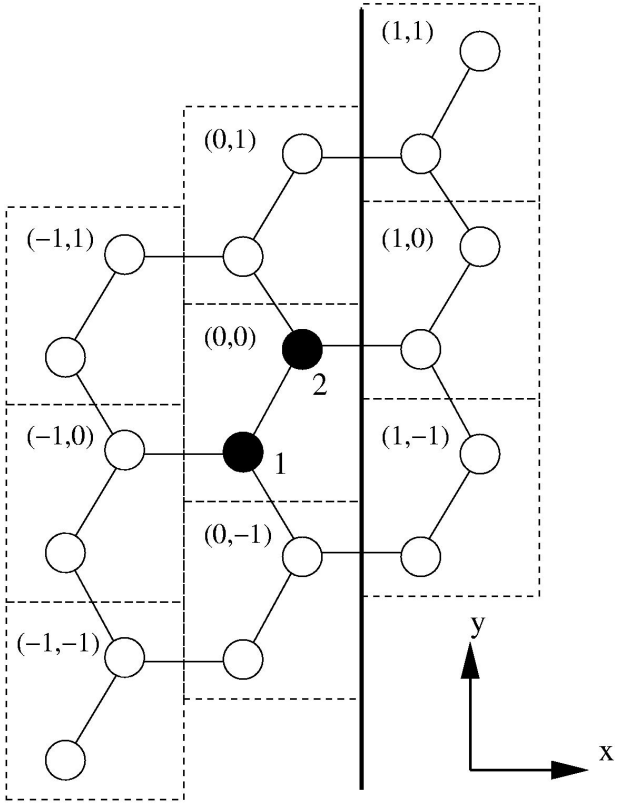
Damping Kernels in Multiple Dimensions

- Damping kernel can be easily computed for any regular crystal lattice across a planar boundary
  - periodicity allows spatial Fourier transform
  - unit cells can be indexed (*l,m,n*) in 3D, or (*l,m*) in 2D
  - boundary condition obtained by solving for atoms just outside boundary (*l*=1) in terms of atoms just inside boundary (*l*=0)
  - final boundary condition has form of **time history integration** with **spatial coupling** along boundary:

$$\mathbf{f}_m^{1\to 0}(t) = \sum_{m'=-\infty}^{\infty} \int_0^t \boldsymbol{\theta}_{m-m'}(t-\tau)\mathbf{u}_{0,m'}(\tau)d\tau$$

  - note that **u** and **f** are vectors containing all dof's in the unit cell, and θ is a matrix coupling them
  - Reference: G. Wagner, E. Karpov and W.K. Liu. *Comp Meth. Appl. Mech. Eng.*, to appear (2004).



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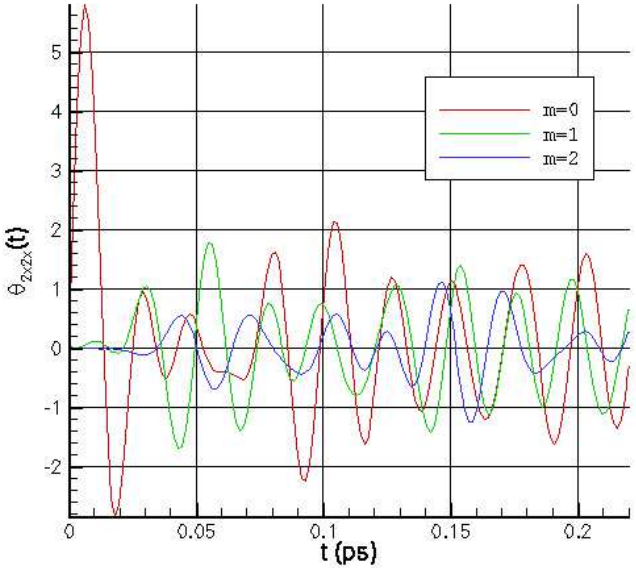
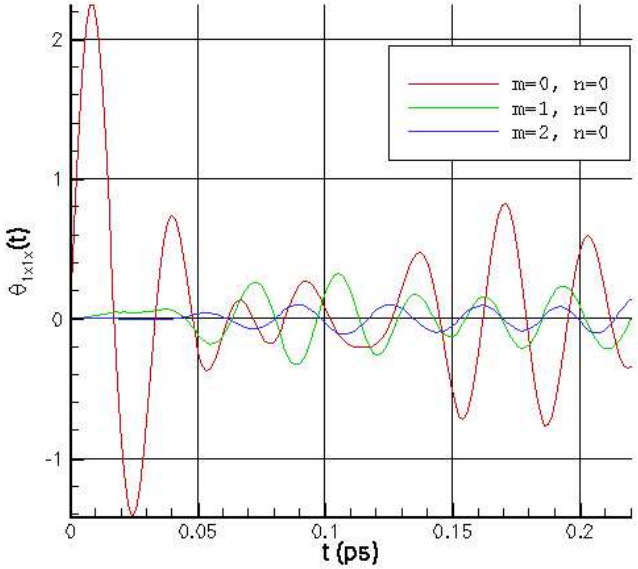
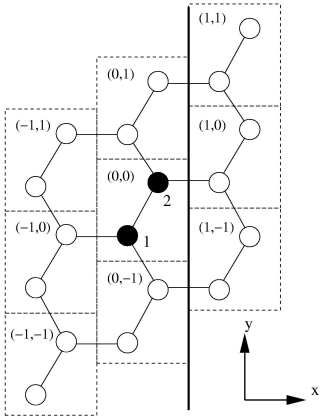
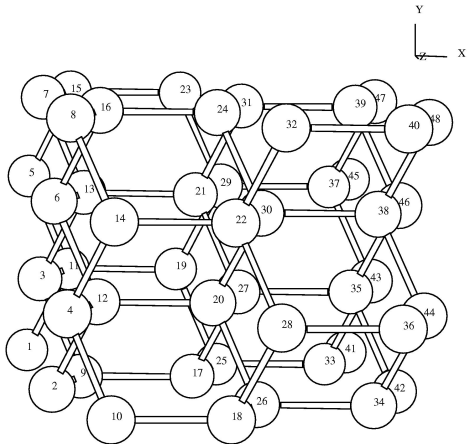
Damping Kernels in 3D: Carbon Structures









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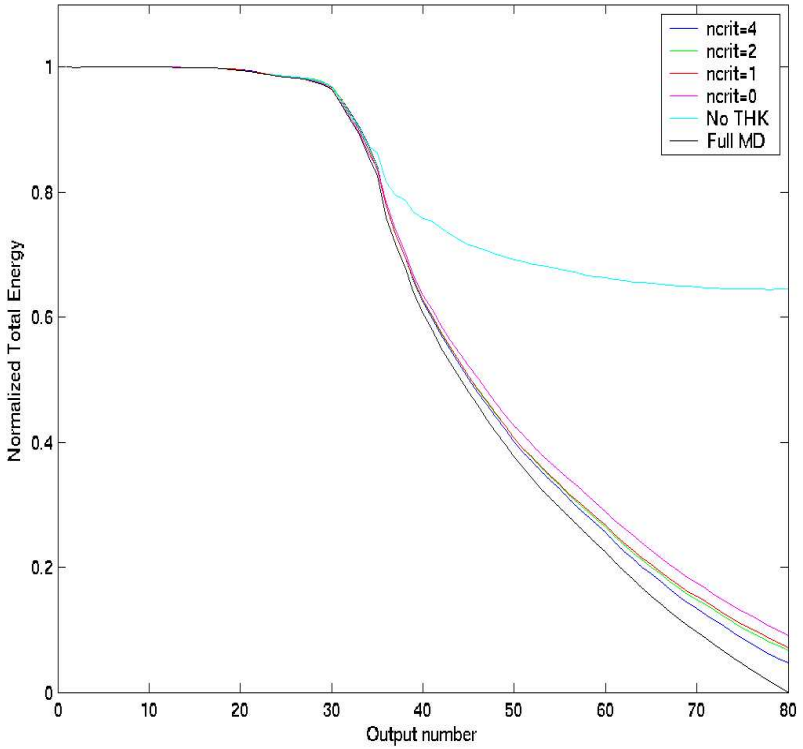
2D Multiscale Wave Propagation

smallnothk.mov

Smallthk.mov



Energy Transfer Rates:

No BC: 35.47%

$N_{crit} = 0$: 90.94%

$N_{crit} = 1$: 92.85%

$N_{crit} = 2$: 93.34%

$N_{crit} = 4$: 95.27%

Full MD: 100%

Harold Park, Northwestern University

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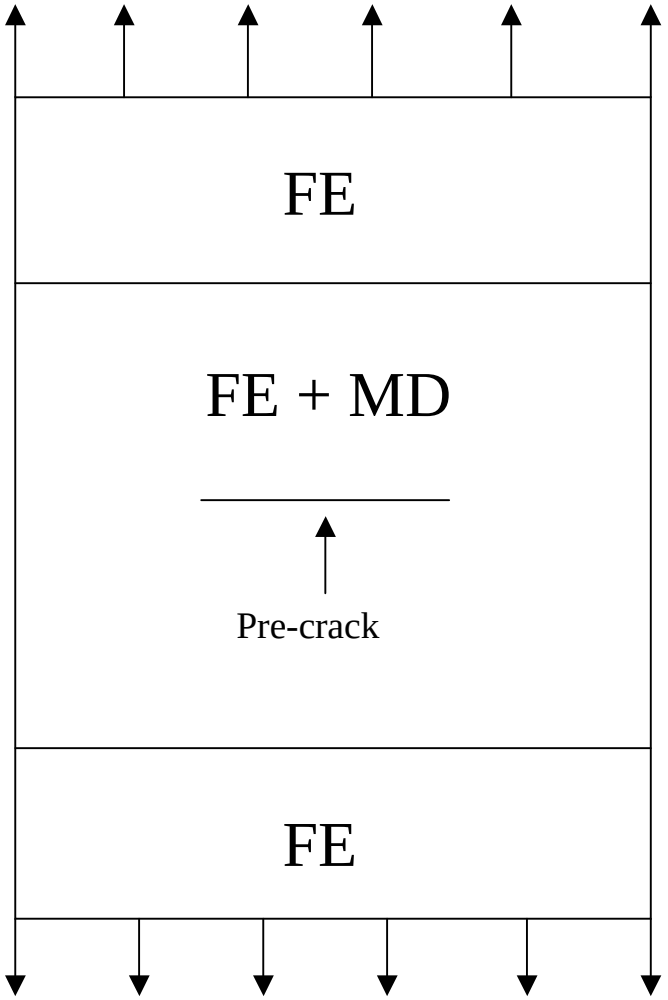
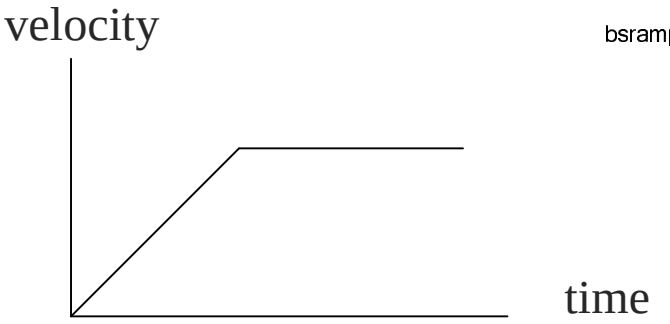
2D Dynamic Crack Propagation



Problem Description:

- LJ 6-12 potential, $\sigma=\varepsilon=1$
- Nearest neighbor interactions
- 90000 atoms, 1800 finite elements (900 in coupled region)
  - 100 atoms per finite element
- $\Delta t_{fe} = 40\Delta t_{md}$
- Ramp velocity BC on FEM
- Full MD = 180,000 atoms

bsrampvel06_301x301_all.mov



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Summary: Coupled MD/FEM

- Bridging scale decomposition allows concurrent simulation of fine scale using MD and coarse scale using FEM
  - bridging scale projection provides a unique decomposition of total solution for separation into coarse and fine scales
  - coarse scale mesh need not correspond to atomic lattice for coupling
  - subcycling can be used to take advantage of the different time scales in the coarse and fine regions
  - coarse scale equations and boundary conditions follow directly from the multi-scale formulation
- Future work:
  - study of approximations in boundary conditions
    - truncations of summations/integrals, approximations to kernel function
  - determination of most accurate/efficient integration of coarse scale region near MD boundary
  - development of coupled energy equation to track fine scale energy
    - time averaging as part of coarse scale projection